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FINAL PROJECT REPORT

MODELING THE DEFORMATION OF ENGINEERED NANO-LAYERED STRUCTURES BY COMPUTER SIMULATIONS
AFOSR AWARD NUMBER F49620-03-1-0031-P00001

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1. Abstract

We developed here fundamental models of plasticity, based on dislocation dynamics and atomistic computer simulation methods for the prediction of the strength and plastic deformation at the nano-to-micro-length scales. The models are applied to the simulation of plastic flow in ultra-strong nano-laminates. The developed methods are: (1) An *ab-initio* based hybrid approach based on an extension of the parametric dislocation dynamics (DD) to bi-materials where the dislocation spreading over the interface is explicitly accounted; (2) a hybrid ab initio-discrete dislocation dynamics model to study the core structure in straight and curved dislocations, with applications to single layers and across material interfaces; (3) Molecular dynamics (MD) modeling of dislocation motion and deformation in nano-layered composite materials and twins; and (4) Dislocation Dynamics (DD) modeling of dislocation motion and deformation modes of anisotropic, nano-layered composite materials. Both coherent and incoherent interfaces have been considered and the lattice resistance of dislocation motion was estimated through the *ab initio*-determined generalized stacking fault energy surface (GSFS). The effects of mismatch in the elastic properties, GSFS, and lattice parameters on the spreading of the dislocation onto the interface and the transmission across the interface have been studied in detail. We find that the competition of dislocation spreading and transmission depends on the characteristics of the GSFS of the interface, and that the strength of can be greatly enhanced by the spreading of the glide dislocation, or by the pre-existence of misfit dislocations. It is shown that interfacial image forces control the plastic deformation and maximum strength of nano-layered materials. The strength of a thin film of alternating nano-layers increases with decreasing layer thickness, up to

a maximum determined by the *Koehler barrier* strength, which results from variation in the Peach-Kohler force across the interface. For alternating Cu/Ni, the maximum strength is estimated to be ~ 1 GPa for a Cu layer thickness of ~ 10 nm, in agreement with experiments. Simulations of the interaction between and edge dislocation and Cu/Ni interface, utilizing the EAM potential, indicate that the dislocation core structure is a strong function of the nano-layer thickness, for laminate periods of less than 20 nm. Results of the atomistic simulations are used in conjunction with DD simulations to establish the deformation modes of nano-layered thin films.

2. Research Objectives

Large-scale computer simulations may provide an additional investigative tool to augment, interpret and plan experimental techniques for mechanical properties at this length scale. The main objective of this proposal is to develop new computational methods for the design of ultra-strong and ductile nano-scale multi-layered material systems. We propose to develop a rigorous methodology for simulating the dynamics of single and collective dislocations for the analysis of plastic flow in multi-layered nano-composites. Dislocation Dynamics (DD) will be used as the main modeling tool. However, the critical parameters required for DD simulations (e.g. Peierls stress, interface resistance and dislocation mobility) are determined by ab-initio and classical MD computer simulations. We have the following goals in the present research:

1. Determine the nature of strength and plastic deformation in nano-scale composites subject to complex stress states.
2. Develop the knowledge base for management of plastic slip in nanolayered composites.
3. Develop large-scale computer simulation tools for *engineering* nanolayered structures. Specific applications to material systems are linked to on-going experimental research.
4. Provide an understanding for the relationships between processing methods and strength.

3. Research Achievements

One of the recent challenges in the race to find new materials for demanding structural and functional applications is the development of ultra-strong, yet ductile material systems. The mechanical behavior of these two types of structures can be vastly different as a result of the particular geometry and structural constraints. Currently, however, the most widely used options for such experimental evaluation have been mainly limited to pointed indenters, scratch-type tests and bulge tests. To interpret these specialized mechanical tests, and to extrapolate to bulk properties for future structural applications, advanced computer modeling and simulations are required. Thus, computer simulation of material behavior has become an indispensable tool, and is now playing an increasingly significant role to complement traditional theoretical and experimental research.

Recent experimental research on the deformation behavior of multi-layer nano-crystal composites shows that very high strength and ductility can indeed be obtained, when plastic deformation is restricted to flow in confined small volumes. New material processing methods, such as wire drawing, sputtering or evaporation, have shown that nano-layered structures can be manufactured to be ultra-strong. The flow stress in nano-layered structures can approach to within 1/3 of the theoretical shear strength of order $\mu/30$, where μ is the shear modulus. In principle, plastic flow can be confined to small volumes by controlling the strength and spacing of *engineered* dislocation obstacles at the nano-scale. However, in practice such confinement is also conducive to plastic flow localization as an easier channel for energy dissipation in the material, rather than storage in elastic and quasi-elastic (i.e. just bowing-out of dislocations) material configurations. It is therefore logical to consider approaches for control and management of plastic flow, as a means of optimizing the required high strength without the spontaneous emergence of possible failure modes. In this research, we address the question of how to control and manage dislocation motion in small volumes with the intent of designing ultra-strong and ductile material systems.

3.1 Dislocation Dynamics in Layered Materials

A variational form of the governing equation of motion for a dislocation loop has been developed for over-damped dislocation dynamics, where the work exerted on dislocation loop expansion is balanced by viscous dissipation [1]. Because the present formulation results in a line integral form of the force vector distribution, it can be readily incorporated into the PDD framework [1]. In this section, we present computer simulation results for dislocation motion in nano-layered materials using the PDD methodology.

Experimental results and isotropic elasticity estimates show that the dominant mechanism that controls the strength and hardness of multi-layer thin films is the influence of the dislocation image force associated with a mismatch in elastic properties between adjacent film layers [2]. For layered materials with a large mismatch in elastic properties, a significant hardness enhancement was observed. On the other hand, for layered materials with small differences in their elastic properties, no measurable hardness enhancement was detected [2]. Two models are often used to explain the observed behavior of hardness (or flow stress) in thin films. In the threading dislocation model [3, 4], the flow stress is determined by the energy balance between the threading glide dislocation segment and the misfit dislocation left behind at the interface. This model results in a flow stress that scales approximately with the inverse of the film/layer thickness. In this model, interfaces are introduced as impenetrable planes for dislocations. The second model is an extension of the well-known Hall-Petch effect. Here, dislocations are assumed to form a pile-up at a boundary until a critical stress is reached. This results in a flow stress, which is inversely proportional to the square root of the layer thickness or grain size. Both

models qualitatively explain the increase in the flow stress with decreasing film/layer thickness, but not the behavior as the layer thickness decreases below tens of nano-meters.

Consider a Cu thin layer (thickness h), sandwiched between two semi-infinite harder Ni substrates. The dislocation is originally located within the thin layer. Cu and Ni are both fcc crystals with [001] out-of-plane orientations and <110>{111} slip systems, and anisotropic elastic constants. In Cu, $|\mathbf{b}|$=0.361 nm, and the dislocation mobility is taken to be isotropic. The system is subjected to a uniform applied biaxial stress. We will ignore here the stress due to lattice mismatch. We only consider the image force effect due to the modulus difference at the Cu-Ni interface. The value of image force increases as the dislocation segment approaches the interface, and is singular exactly at the interface. We assume also here that dislocations do not dissociate into partials, and take the cut-off radius to be $r_0 \sim$ b. Detailed atomistic simulations are required to ascertain the value of the cut-off distance. In the following simulations, we assume that there is one Frank-Read (F-R) source inside one of the layers, and that the source dislocation is initially straight and pinned from both ends.

Confined Layer Slip (CLS)

Figure (1) shows the propagation mode of a source dislocation in a Cu layer of thickness 144 nm at different loading levels. We choose the length L of the original dislocation to be longer than the layer thickness, h, i.e. L=4h. Under a small applied stress below a critical value (approximately estimated by Freund's formula, the dislocation will bow out in the Cu layer towards the interface. As a result of the image force exerted by the harder Ni layer, the dislocation is repelled away from the interface and reaches an equilibrium configuration. If the applied stress is larger than the critical value, the dislocation first bows out towards the interface, then it is blocked by the image force and is confined to propagate within the layer.

Loss of Slip Confinement

As individual layers become very thin (i.e. in the tens of nanometers), only single dislocations can propagate and expand upon the application of an externally applied stress. However, because the layer thickness is very small, the curvature of the dislocation loop in segments subtended between layers would be extremely high, and thus self-forces

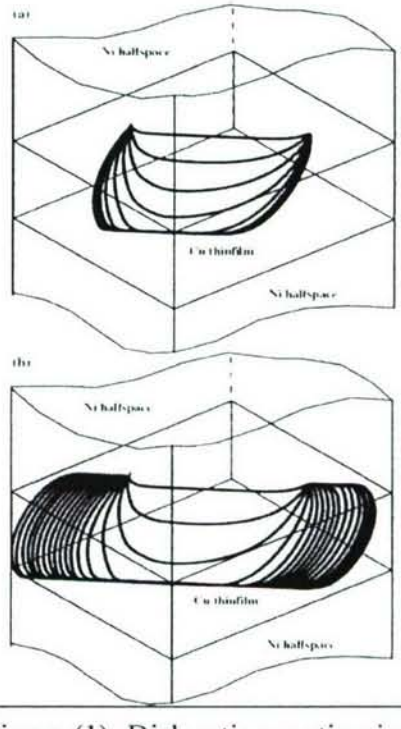

Figure (1): Dislocation motion in a thin layer with h=144 nm under different applied biaxial stress levels (a) σ_a=210 MPa, σ_c =250 MPa, and (b) σ_a=280 Mpa. Each line corresponds to a time increment of 0.1 ns.

in these regions are very substantial. The externally applied stress would have to overcome such large self-forces if these curved segments are to expand. The applied P-K force on those segments that are parallel to the interface does not have to overcome self-forces because the curvature of these segments is small. Rather, the image force from neighboring and other interfaces would have to be overcome by the applied P-K force. Since we regularized the solution by selecting a cut-off radius of one Burgers vector on either side of the interface, the dislocation will be repelled with a maximum image force on one side of the interface, and then attracted with a different maximum force once it crosses the interface. If the applied stress is high enough that the maximum P-K force on the straight dislocation segments close to the interface overcomes both repulsive and attractive forces, the dislocation will cross from one layer to the neighboring one, and CLS is finally lost, as shown in Figure (2).

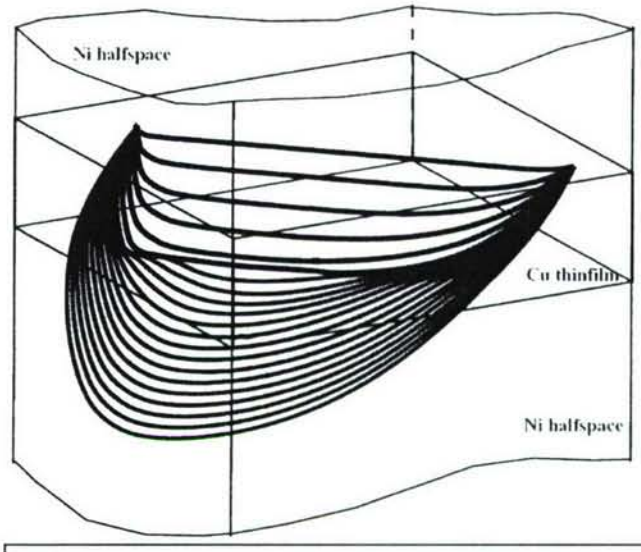

Figure (2): Loss of dislocation confinement at high applied stresses in nano-layered materials.

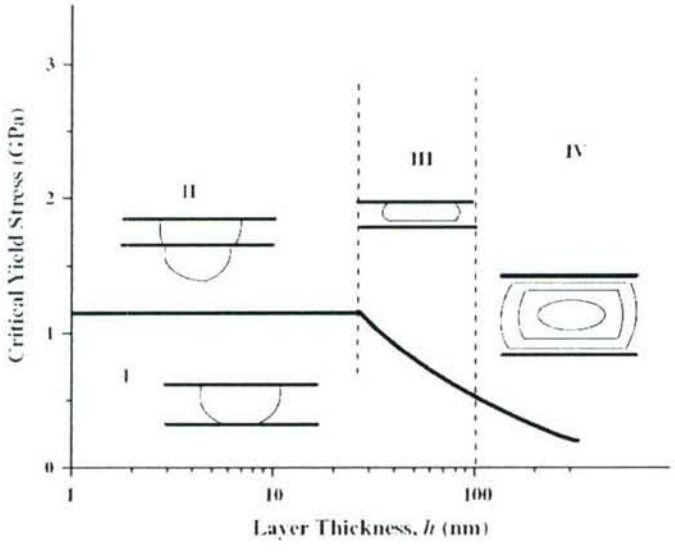

Figure (3): Deformation map for nano-layered materials.

Figure (3) shows results of our calculations for the maximum strength of a copper layer in a thin film of alternating Cu/Ni layers based on the activation of a single F-R source, as a function of the layer period. Experimental results for nano-indentation by Misra et al. [5] and Clemens et al. [1] are also shown. Since Freund's formula [3] is often used to estimate the strength of thin films, film strength using this formula is also shown as a solid line on the same figure for comparison. For layers of thickness less than approximately 100 nm, a single F-R

source will determine the overall strength of the layer as a competition between confinement in the layer by image forces generated by elastic modulus mismatch, and resistance to deformation by self-forces on the curved ends of the dislocation loop. If the modulus mismatch is not too great, dislocation loops will cross from layer to layer rather than be confined within a layer. One would expect that the maximum strength be determined by the layer thickness and the ratio of elastic modulii as well. For thicker layers, F-R sources can operate many times leading to dislocation multiplication and the formation of a pile-up. In such case, the dominant deformation mode is the Hall-Petch mechanism.

Conclusions

The following conclusions are drawn from the present work:

1. The influence of free surfaces or interfaces on dislocation motion through image forces extends into the material to several hundred-lattice constants.
2. In thin anisotropic films containing many layers of small thickness, interaction between several interfaces contributes to the image force on dislocations. No simple geometric image construction can be found to yield accurate magnitude and direction of interface image forces.
3. In thin Al films on Cu substrates, it is shown that a small layer of aluminum oxide can reverse the surface image force from attractive to repulsive. If the oxide film thickness is greater than the film thickness itself, its image force can be approximated by the semi-infinite half-space results.
4. Plastic deformation of very thin layers in the tens of nm thickness range is controlled by a competition between the resistance of curved segments due to high self-forces, and the maximum force to transmit nearly straight segments across the interface (i.e. the Kohler barrier). If the layer is too thin, this results in high curvatures and resistance to CLS. Depending on the ratio of the elastic modulii of adjacent layers, dislocations may find an easier path to move into adjacent layers, and thus CLS is lost. On the other hand, if the ratio of elastic modulii between adjacent layers is sufficiently high and the layer thickness is sufficiently large, dislocations are confined within one layer.
5. Strength calculations from the present model show reasonable agreement with experimental nano-indentation data on Cu/Ni nano-layered materials. Strength saturation below layer thicknesses of ~ 20 nm is a result of the near independence of the Koehler barrier strength on layer thickness.
6. Four general deformation mechanisms are identified for layered thin films: quasi-elastic, plastic instability, Confined Layer Slip, and the Hall-Petch regime, consistent with recent literature.

3.2.Hybrid Ab Initio-DD Model for Dislocation Core

The GSFS (γ-surface) can be interpreted as the two-dimensional energy profile when the two crystal halves above and below the glide plane are shifted rigidly against each other by a constant fault vector, $\boldsymbol{u}$, and the atoms are allowed to relax perpendicular to the glide plane. For a fault vector $\boldsymbol{u}$ there is an interfacial restoring stress $\mathbf{F}_r(\mathbf{u}) = -\nabla(\gamma(\mathbf{u}))$, which has the same formal interpretation as the restoring stress in the Peierls-Nabarro (PN) model. The electronic structure calculations of the GSFS were done using the projector augmented-wave (PAW) method as implemented in the VASP code. The *ab initio*-determined GSFS projected along the [121] direction for the pure Cu and Ni and along the [001] direction for the Cu/Ni interface are shown in Figure 4. The first energy maximum encountered along the[121] direction for the Cu and Ni is the unstable stacking fault energy (γ_{uns}) which represents the lowest energy barrier to nucleate a dislocation from a crack tip The first energy maximum encountered along the [121] direction for the Cu and Ni is the unstable stacking fault energy which represents the lowest energy barrier to nucleate a dislocation from a crack tip at 0 K. The local minimum on the other hand, corresponds to the intrinsic stacking fault energies (γ_{intrin}). The calculated values of γ_{uns} are 225 mJ/m^2 and 350 mJ/m^2 for Cu and Ni, respectively, while the values of γ_{intrin} for Cu and Ni are 53 mJ/m^2 and 163 mJ/m^2, respectively. As expected, the GSFS of the interface is symmetric along the [110] direction and it has unstable stacking fault energy of 730 mJ/m^2, which is much higher than the corresponding value of Ni and Cu. The absence of a saddle point in the GSFS of the interfaces suggests that the full dislocation on the interface does not dissociate.

The PN model has been modified to investigate the strengthening mechanisms in slipping and rigid Cu/Ni bimaterial. The effects of the mismatch in the elastic properties, the mismatch in the GSFS, the mismatch in the lattice parameters and the existence of misfit dislocations are explicitly taken into account. For slipping interface, part of the dislocation content can be accommodated by the interface through dislocation spreading. Any dislocation moves from the glide plane to the core that

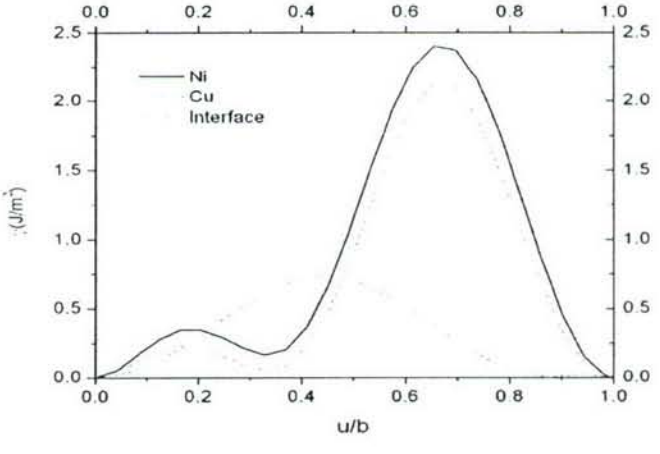

Figure 4 *Ab initio stacking fault energies for Ni and Cu along the [112] direction and for the interface along [100] direction.*

interface is divided into two identical fractional dislocations, symmetrically placed with respect to the slip plane. In particular, the mismatch in lattice constant between Cu and Ni is accommodated by the fractional residual slip on the interface. The continuity of the Burgers vector requires that:

$$b_{Cu} = n_{Cu} db_{Cu} + n_{Ni} db_{Ni} + 2n_{Int} db_{Int}, \qquad (1)$$

where $N = n_{Cu} + n_{Int} + n_{Ni}$, n_{Cu}, n_{Ni}, n_{Int} are the number of fractional dislocations in Cu, Ni, and interface, respectively, and $db_{Cu} = \frac{b_{Cu}}{N}$, $db_{Ni} = \frac{b_{Ni}}{N}$, and $db_{Inti} = \frac{b_{Cu}}{2N}$.

For the Cu/Ni bimaterial problem, the equilibrium condition of a fractional dislocation *i* depends on whether the fractional dislocation is in Cu, Ni or on the interface. The total force on a fractional ***screw*** dislocation *i* is the sum of the stress exerted on the fractional dislocation from other fractional dislocations located in Cu, on the interface, and in Ni, respectively, the lattice restoring force derived from the GSFS, and the coherency stress. The large increase in the mechanical strength of nano-layered materials is widely attributed to the presence of interfaces. Several factors can affect the mechanical and physical properties of the interface such as: the unstable stacking fault energy of the interface, γ_{int}, which is a measure of the propensity of interfacial sliding and which is directly related to the electron charge bonding across the interface, the presence of misfit dislocations, and the presence of impurities. The smaller γ_{int} is, the easier is for the interface to slide, thus allowing the dislocation to spread onto the interface.

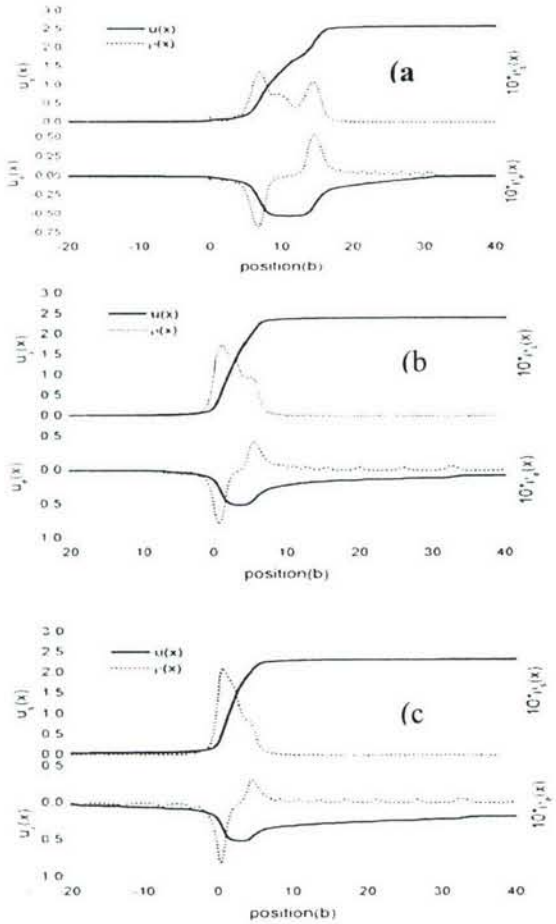

Figure 5: the displacement u(x) and density ρ(x) profiles for the dislocation as it moves from cu towards Ni. The GSFS of the interafce is equal to the ab initio value.

Figure 5 shows the equilibrium edge and screw displacement and the corresponding Burgers vector density ρ(x) of the dislocation for three values of applied stress. The edge and screw Burgers vector density are defined by $\rho_e(x) = du_e/dx$, and $\rho_s(x) = du_s/dx$. The screw dislocation, originally placed in the soft material (x>0) is pushed towards the Cu/Ni interface. For relatively low values of applied stress (around 2.0 GPa), the dislocation core in Cu dissociates into two partials bounding a stacking fault with a separation distance of about 7b (figure 5a). As the external stress

increases, the dislocation approaches the interface but remains dissociated. However; the dislocation core structure has changed significantly. First, the dislocation Burgers vector density accumulates on the leading partial at the expense of the trailing partial (figure 5 b,c). Second, the dislocation core constricts steadily and the two partials become significantly overlapped (figure 5c). Note, that the maximum value of the screw component of the displacement in Cu is 2.35 Å, while the Burgers vector of Cu is 2.6 Å. This reduction of Burgers vector is a result of the energetically favorable spreading of the core onto the interface. Our results suggest that the dislocation spreading process proceeds via the following mechanism: When the leading fractional dislocation reaches the vicinity of the interface it spreads on it, if it is energetically favorable. As the external stress is increased, the trailing fractional dislocations follow and spread onto the interface. The spreading process continues until the interface can no longer accommodate additional slip. At the critical value of the applied stress, once the leading dislocation on the glide plane overcomes the interfacial barrier and is transmitted to the Ni crystal, the remaining fractional dislocations follow.

In figure 6 we show the time evolution of the displacement u(x) and the Burgers vector density profiles $\rho_s(x)$ and $\rho_e(x)$ of the dislocation when the applied stress has reached its critical value of 3.35 GPa. At the initial stage of the dislocation transmission process, most of the fractional dislocations are localized in the vicinity of the interface in the Cu host (figure 6a).

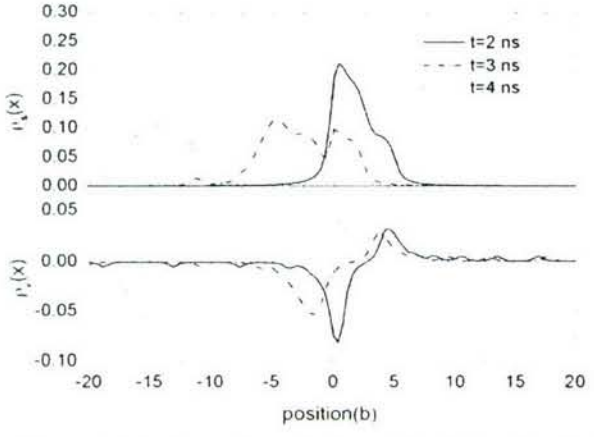

Figure 6 The dynamic evolution of the dislocation during the transmission process. The critical stress for penetration is 3.35 GPa and as the simulation time passes, the dislocation penetrates to Ni.

As the fractional dislocations relax, they get transmitted through the interface towards the Ni host till all of them pass. Note that after the dislocation gets transmitted, the density profile shows the formation of two partials with a separation distance of about 6b (figure 6c). The peak in the density profile at x=0 indicates the formation of a ledge on the interface, in agreement with MD simulations for edge or mixed dislocations for the Cu/Ni interface.

Interfaces can be coherent, semi-coherent or fully non-coherent. In the case of fully non-coherent structures, dislocation motion is restricted to individual layers, i.e. the interface acts as a dislocation sink. For a semi-coherent interface as in the case of Cu/Ni, the dislocation transmission across the interface is possible depending on the stacking fault energy of the

interface. In order to explore the effect of interfacial sliding on the critical stress required for dislocation transmission, we have varied the value of γ_{int} with respect to its *ab initio* value γ^{ab}_{int} =730 mJ/m^2. The spreading of fractional dislocations on the interface imposes an extra energy barrier on the transmission of the glide dislocations. The extra barrier is due to the repulsive elastic interactions between the glide and interfacial fractional dislocations and the formation of the interfacial ledge which hinders the transmission process from Cu to Ni. Consequently, the critical value of applied stress for dislocation transmission increases (decreases) to the value of 4.2 GPa (3.2 GPa) as the interfacial GSFS decreases (increases) compared to its corresponding *ab initio* value. Ledge formation is partially due to the accommodation of the misfit in the Burgers vector between Cu and Ni which is about 0.10 Å. The variation of the critical shear stress with the GSFS of the interface is shown in Figure 5 above. A rigid interface does not accommodate core spreading and therefore it is not affected by the change in interfacial GSFS. The removal of the edge component leads to a significant increase in the transmission stress for the slipping interface case and minor increase for the rigid interface case.

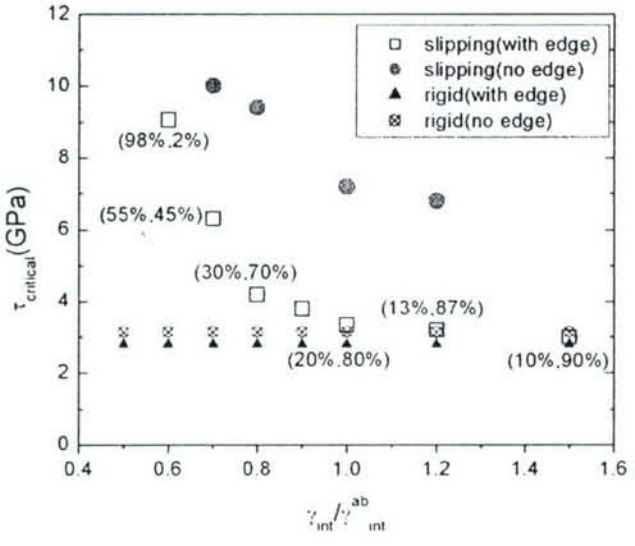

Figure 7. *The variation of the critical shear stress with the GSFS of the interface. Rigid interface does not accommodate core spreading and therefore it is not affected by the change in interfacial GSFS. The removal of the edge component leads to a significant increase in the transmission stress for the slipping interface case and minor increase for the rigid interface case.*

3.3 Nonsingular Descriptions of Dislocation Core: A Hybrid Atomistic-Continuum Approach

We have developed a hybrid approach for the core structure of straight and curved dislocations that links the parametric dislocation dynamics method with ab initio calculations. The hybrid approach is an extension of Peierls-Nabarro (PN) model that takes into account all

three components of atomic displacements of the dislocation and utilizes the entire generalized stacking fault energy surface (GSFS) to capture the essential features of dislocation core structure. The method combines the commonly used dislocation dynamics (DD) approach for direct interaction and motion of dislocations with the atomic calculations for the lattice restoring forces. These forces are extracted from the GSFS calculated from first-principles density functional theory (DFT). We have investigated the presence and absence of planar dissociation are investigated for two FCC lattices, aluminum (Al) and silver (Ag). For straight dislocations, the results from the proposed model are shown to be in excellent agreement with the existing literature for both Al and Ag. For dislocation loops, the core structure is obtained based on simplified assumptions. In contrast to the undissociated dislocation loops in Al, it is found that the core width and the partial separation typically vary along the angular direction measured with respect to the Burgers vector direction in Ag. The method is computationally inexpensive and can be easily implemented to solve an important class of problems with minimum commitment to atomic details as discussed.

Dislocations play a central role in understanding many key phenomena in materials science and engineering. The traditional description of elastic field and energies of dislocations is based on continuum theory of linear elasticity that suffers from long-standing problem of singularities at the dislocation center. Singular solutions are often circumvented by introducing an artificial core-cutoff radius. This limits the applicability of the theory to describe situations where it is important to know the strained state and nanoscopic details within a few atomic spacing surrounding the dislocation center, known as the dislocation core. There has been a great deal of interest in describing accurately the dislocation core structure on an atomic scale and providing a non-singular treatments because of its important role in many phenomena of crystal plasticity.

Computational methods based on direct atomistic simulations using either empirical interatomic potentials or *ab initio* calculations have been used to understand the core properties [15,16]. Empirical potentials involve the fitting of parameters to a predetermined database and hence may not be reliable in predicting the core properties of dislocations, where severe distortions like bond breaking, bond formation and switching necessitate a quantum mechanical description of the electronic degrees of freedom. *Ab initio* total energy calculations, though considerably more accurate, extended systems, such as dislocation cores, are far too large to be directly studied in this way due to computational limitation. On the other hand, continuum methods based on the PN framework have been subject of various studies due to their simple and easily tractable hybrid nature, which essentially establishes a connection between atomic and continuum length scales and offers an attractive alternative to the large-scale atomic simulations.

Computational methods based on continuum models to treat dislocation loops of arbitrary shape are rather sparse. A variational boundary integral method has been used for the analysis of three-dimensional cracks with arbitrary geometry by representing them as continuous distributions of

dislocation loops. The PN model enters into this approach by refining the sinusoidal restoring stress law to study the homogeneous nucleation of dislocations from crack tips, and the slip distribution is obtained by minimizing the total energy. As a result, the model have not been used for the crystals those are highly dissociative in nature.

We have developed a simpler and more pragmatic approach based on direct interaction and motion of dislocations, known as dislocation dynamics. Developed over the past two decades, DD is a direct approach that attempts to simulate the aggregate behavior of large dislocation ensembles and holds considerable promise for uncovering the microscopic origins of crystal strength. In the model presented in this work, we have utilized this powerful tool to obtain the core structure of the original dislocation which is represented by arrays of Volterra dislocations of *infinitesimally* small Burgers vector. The core structure is determined by seeking equilibrium configuration of these fractional dislocations via force balance. In general, for a dislocation of 3D geometric shape these forces are of four types: (1) applied external forces (2) long-range interaction forces with other dislocations (3) self-forces as a result of curvatures on defect surfaces, and (4) lattice restoring forces that control separation or sliding across the glide plane, and are determined from the γ surface. The major advantage of the proposed model is that the interaction force terms for Volterra dislocations are readily available for a number of classic problems, e.g., dislocation transmission across interfaces, dislocation interaction with a precipitate, dislocation cross slip, etc.

In Fig. 8, we compare the dislocation density for screw and 30° dislocations. Noticeably, a full screw dislocation tends to dissociate in two 60° partials. The partial separation distance we obtained from the model calculation is in an excellent agreement with the TEM measurement and SVM calculations reported earlier for that in Ag, which is about 20°. Obviously, the lack of a clear dissociation in Al results from the fact that the intrinsic stacking fault energy in Al is much higher than that in Ag.

The dissociative nature of a dislocation loop in Ag is studied with the goal to approximately understand the nature of the partial separation. A uniform shear stress is applied along the [101] direction (chosen as the x-direction) and the equilibrium configuration of the loop arrays is obtained. The magnitude of the applied stress is 525 MPa and the equilibrium configuration of the fractional dislocation loops is obtained. From the equilibrium configuration, the slip displacement, u, can be constructed in a trivial manner as discussed earlier. The density of the slip displacement component u_x along the radial direction can now be plotted as shown in Fig. 6(b). A clear separation between the two groups of partials is obtained in case of Ag. Noticeably, the structure of the edge component of the core, which is along the partial Burgers vector direction for each group, is wider than the screw component.

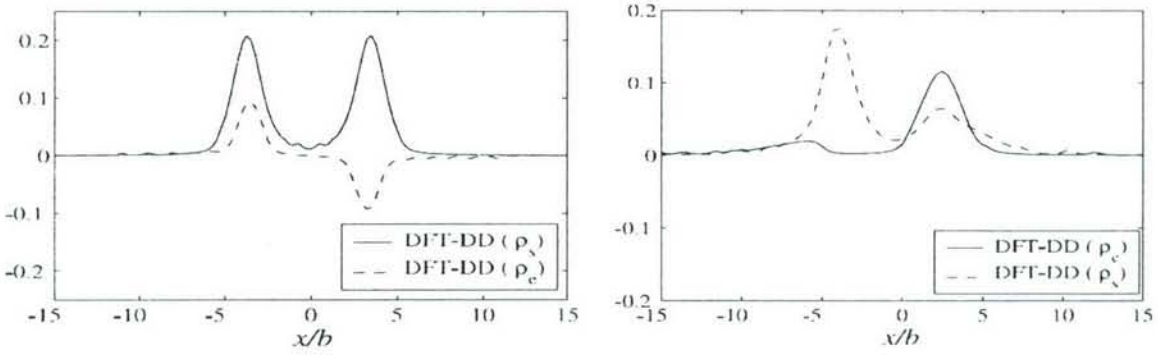

Figure 8 Dislocation density for (a) an edge dislocation and (b) a 60° dislocation obtained from the two models. The DFT γ surface is used in both cases.

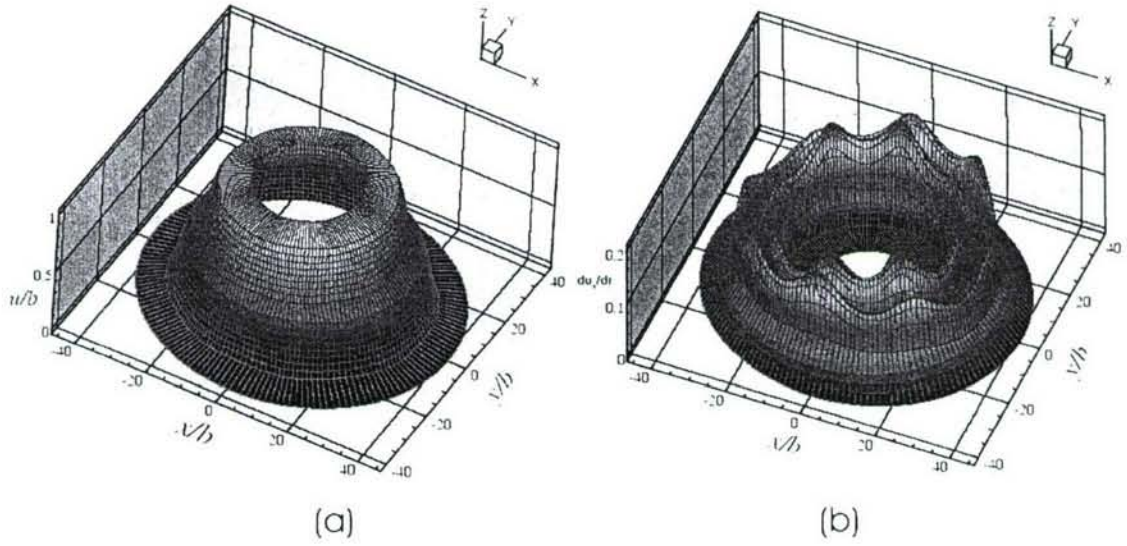

Figure 9 *(a) The 3D representation of the core structure as a function of the slip displacement, u_x, obtained from the equilibrium configuration of the loop arrays under an applied shear stress level of 525 MPa (b) Dislocation density obtained from the equilibrium configuration.*

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6. Personnel Supported

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7. Publications

1. Nasr M. Ghoniem, "From the Nano to the Macro with Parametric Dislocations: Investigations of Dislocation Cores, Plasticity and 3-D Fracture ", *Proc. The 2nd International Conference on Multiscale Materials Modeling (MMM-2),* Los Angeles, CA., U.S.A., October 11-14, 2004, Nasr M. Ghoniem, Editor, Page 265-267.

2. S. Banerjee, N.M. Ghoniem, and N. Kioussis,"A Computational Method for Determination of the Core Structure of Arbitrary-shape 3D Dislocation Loops ", *ibid,* Page 23-25.
3. Lan Li, and Nasr Ghoniem, "MD Simulations of Dislocation Core Transmission Across Interfaces in Nanolayered Cu-Ni," ibid.
4. A. Coho, N. Kioussis, N.Ghoniem, "Dislocation properties of Ni-Cu nanolaminates," ibid.
5. N.M. Ghoniem & N. Kioussis, "Hierarchial Models of Nanomechanics and Micromechanics," *Handbook of Theor. & Comp. Nanotechnology ;* Edited by Michael Rieth and Wolfram Schommers, American Scientific Publisher,**Volume 1:**, Pages (1–97)(2005).
6. Xueli Han and Nasr M. Ghoniem, "Stress Field and Interaction Forces of Dislocations in Anisotropic Multilayer Thin Films," *Phil. Mag.*, **85(11)**1205-1225 (2005).
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8. M.A. Shehadeh, G. Lu, S. Banerjee, N. Kioussis, and N.M. Ghoniem, "Dislocation transmission across Cu/Ni interface" Phil. Mag. 2006, In Press.
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10. Ghoniem & Walgraef, "Self-organization & Instabilities in Materials: Vol. I – Fundamentals, Vol. II - Applications" Oxford Press, 1100 pages, In Press, 2007.

8. Awards Received

(1) N.M. Ghoniem, selected General Chair of the Second International Conference on Multiscale Modeling, Los Angeles, CA., October 11-16, 2004 (see http://www.multiscalemodeling.com/).
(2) N.M. Ghoniem, Invited Lecturer, Gordon Conference on Physical Metallurgy, Holderness School, New Hampshire, July 2004.
(3) N.M. Ghoniem, Invited Lecturer, NSF-sponsored Advanced Materials South America Workshop, Rio de Janeiro, Brazil, August 2004.
(4) N.M. Ghoniem, Elected Fellow of the American Society of Mechanical Engineers (ASME).
(5) Kioussis, Director of Third International Worskshop of Strong Correlations and Materials Properties, Kos, Greece, June 2004.
(6) Kioussis, KITP fellow in the Institute of Theoretical Physics, UCSB, 2005-2007.

9. Transitions

None